PLS Mean Centering

Partial Least Squares (PLS) with Mean Centering

Partial least squares usually uses mean-centered data to compute C_{pls} using the weights from the SIMPLS algorithm with r latent variables.

```
X = A_train;
Y = C_train;

X0 = X - mean(X,1);
Y0 = Y - mean(Y,1);
[X_loadings, Y_loadings, X_scores, Y_scores, Weights] = pnnl_simpls(X0, Y0, r);

B_pls = Weights * Y_loadings';

C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
```

Partial Least Squares (PLS) without Mean Centering

The following is PLS without mean centering.

```
X = A_train;
Y = C_train;

[X_loadings,Y_loadings,X_scores,Y_scores,Weights] = pnnl_simpls(X,Y,r);

B_pls = Weights * Y_loadings';

C_pls = A_unknown * B_pls;
```

Combined algorithm

To make it easier to run with the rest of the tools in the PNNL toolbox, we combined mean-centered and non-mean-centered into one function with `meanCentered` as an optional argument. When `meanCentered` is not used as an input, then the default is to compute without mean-centered data.

```
function [C_pls, B_pls] = pnnl_pls(A_train, C_train, A_unknown, r, meanCentered)
     if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [X_loadings,Y_loadings,X_scores,Y_scores,Weights] = pnnl_simpls(X0,Y0,r); %#ok<ASGLU>
```

```
        B_pls = Weights * Y_loadings';

        if meanCentered
            C_pls = (A_unknown - mean(A_train,1)) * B_pls + mean(C_train,1);
        else
            C_pls = A_unknown * B_pls;
        end
    end
```

Napalm Data

Load the included napalm data to run the PLS algorithms.

```
clearvars
load pnnl_napalm_data
whos
```

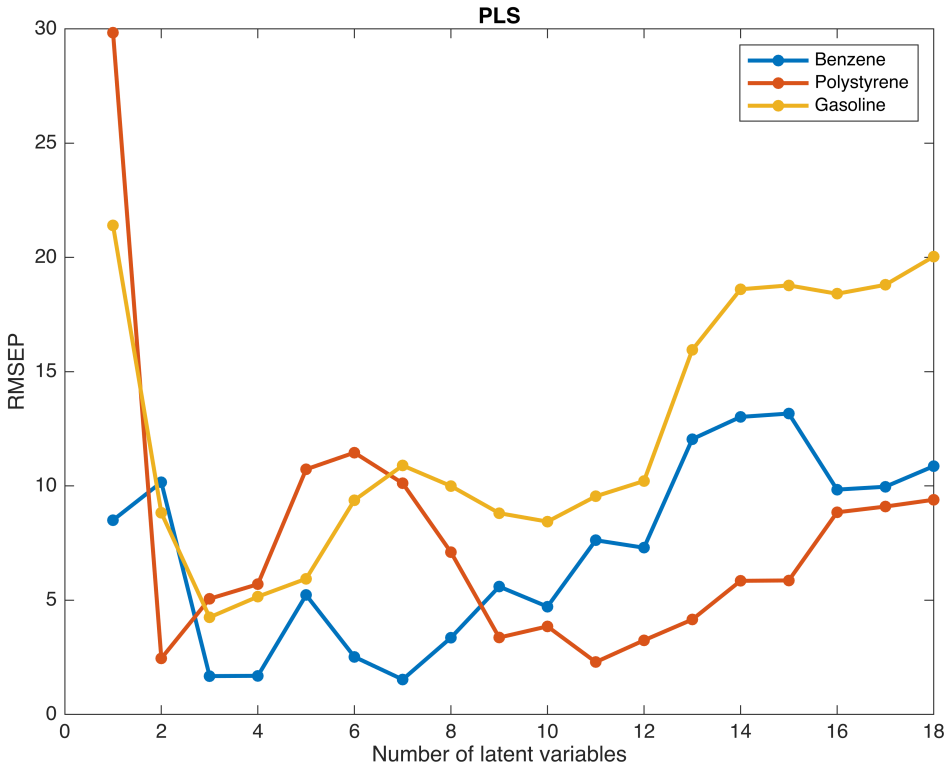
```
  Name                    Size                Bytes  Class     Attributes

  A_train                20x1713            274080  double
  A_unknown              12x1713            164448  double
  C_train                20x3                  480  double
  C_validation           12x3                  288  double
  ConcentrationUnits      1x4                    8  char
  ConstituentNames        1x3                  364  cell
  WavenumberLabel         1x20                  40  char
  Wavenumbers             1x1713             13704  double
  ans                     1x1                    8  double
```

Optimal number of latent variables for PLS with mean centering

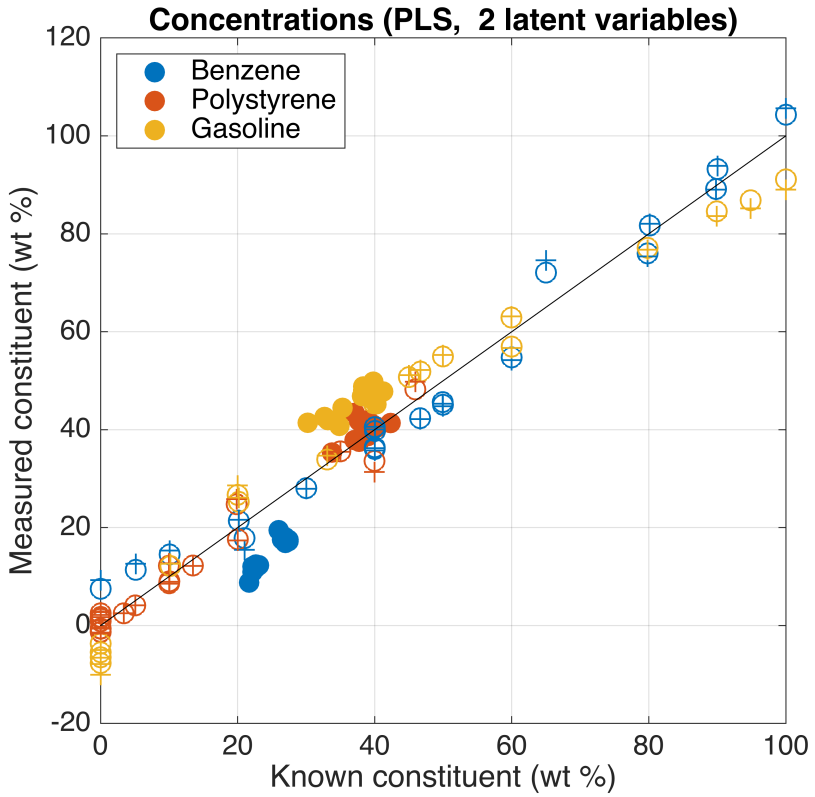
Compute PLS with mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = true;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



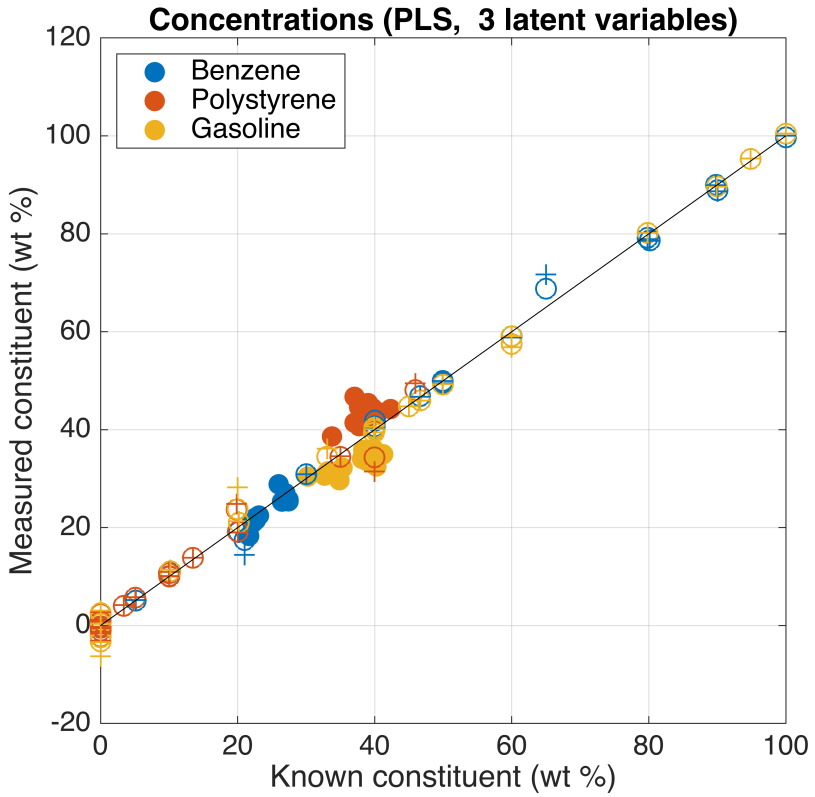
For mean-centered data, it looks like the knee in the curve for polystyrene is 2 latent variables, and 3 for benzene and gasoline. Plot them to see what they look like.

```
nLatentVariables = [2,3];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 2 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1479	2.296	5.5014
RMSECV	5.0229	2.924	6.5258
RMSEP	10.164	2.4566	8.8266

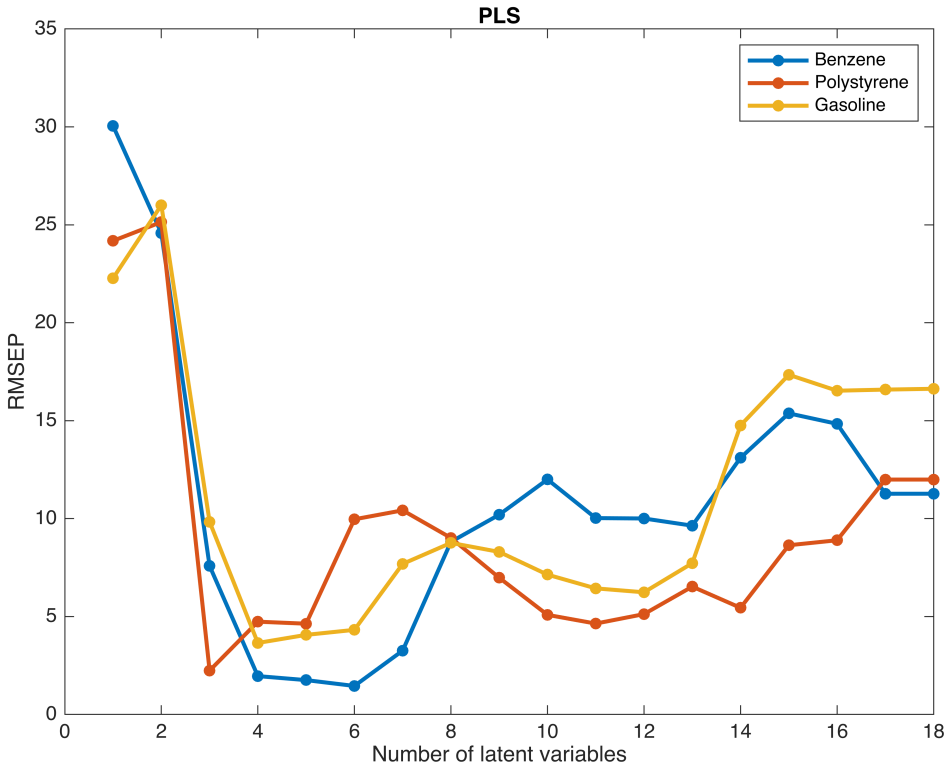



```
Legend: Dot is predicted. Circle is train. Cross is cross-validation.
--------------------------------------------------------------------------
  PLS,  3 latent variables       Benzene    Polystyrene       Gasoline
                    RMSEC        1.3968         1.8465         1.5789
                   RMSECV        2.2406         2.6176         2.7657
                    RMSEP        1.6799         5.0647         4.2528
--------------------------------------------------------------------------
```

Optimal number of latent variables for PLS without mean omentering

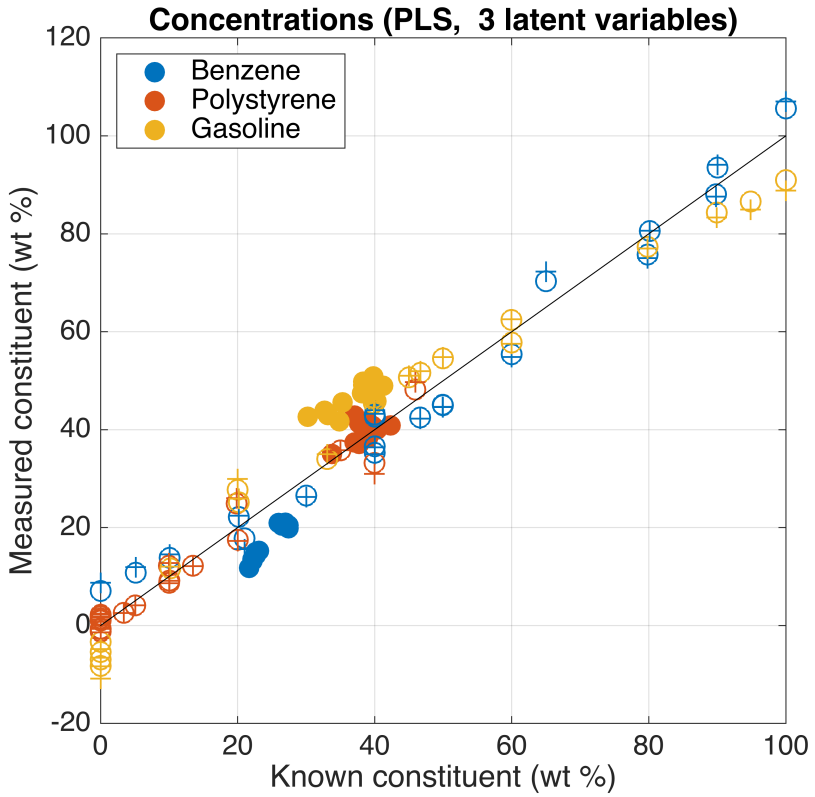
Compute PLS witout mean centering for 1 through 18 latent variables and plot RMSEP for them.

```
nLatentVariables = 1:18;
meanCentered = false;
[C_pls, RMSEP_pls] = pnnl_napalm_pls(nLatentVariables,meanCentered);
plot(nLatentVariables, RMSEP_pls,'.-','LineWidth',2,'MarkerSize',20)
xlabel('Number of latent variables')
ylabel('RMSEP')
title('PLS')
legend(ConstituentNames{:})
```



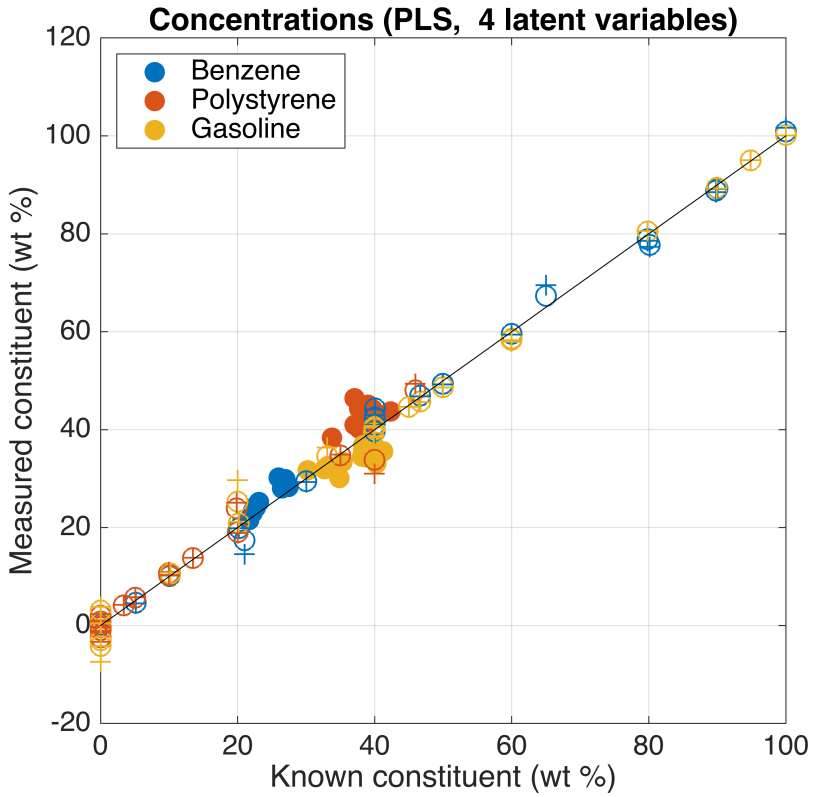
Without mean centering, it looks like the knee in the curve for polystyrene is 3 latent variables, 4 for gasoline, and 6 for benzene. Plot them to see what they look like.

```
nLatentVariables = [3 4 6];
pnnl_napalm_pls(nLatentVariables,meanCentered);
```



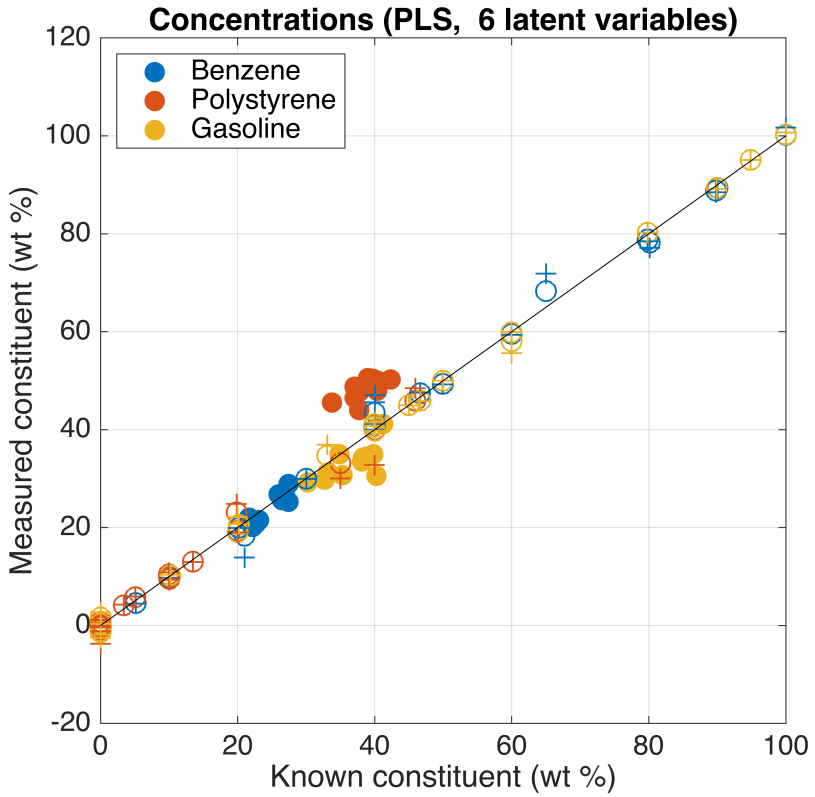
Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 3 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	4.1853	2.3592	5.6109
RMSECV	5.0232	2.9897	6.6976
RMSEP	7.5851	2.2404	9.8369



Legend: Dot is predicted. Circle is train. Cross is cross-validation.

PLS, 4 latent variables	Benzene	Polystyrene	Gasoline
RMSEC	1.6636	1.921	1.9509
RMSECV	2.3112	2.6884	3.2095
RMSEP	1.9599	4.7379	3.6527




```
Legend: Dot is predicted. Circle is train. Cross is cross-validation.
------------------------------------------------------------------------
  PLS,  6 latent variables       Benzene   Polystyrene      Gasoline
                    RMSEC        1.4134       0.99256       0.91242
                   RMSECV        3.1544        2.5526        1.7502
                    RMSEP        1.4567        9.9656        4.3211
------------------------------------------------------------------------
```

```
%#ok<*ASGLU>
```

operated by

BATTELLE

for the

UNITED STATES DEPARTMENT OF ENERGY

under Contract DE-AC05-76RL01830